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Existence of Weak Solutions for the Cahn-Hilliard Reaction Model Including Elastic Effects and Damage

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Abstract. In this paper, we introduce and study analytically a vectorial Cahn-Hilliard reaction model coupled with rate-dependent damage processes. The recently proposed Cahn-Hilliard reaction model can e.g. be used to describe the behavior of electrodes of lithium-ion batteries as it includes both the intercalation reactions at the surfaces and the separation into different phases. The coupling with the damage process allows considering simultaneously the evolution of a damage field, a second important physical effect occurring during the charging or discharging of batteries.

Mathematically, this is realized by a Cahn-Larch system with a non-linear Newton boundary condition for the chemical potential and a doubly non-linear differential inclusion for the damage evolution. We show that this system possesses an underlying generalized gradient structure which incorporates the non-linear Newton boundary condition. Using this gradient structure and techniques from the field of convex analysis we are able to prove constructively the existence of weak solutions.

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Key Words: Cahn-Hilliard reaction system; rate-dependent damage; phase separation; existence; non-linear Newton boundary condition.

1 Introduction

Lithium-ion batteries belong to the most promising technologies to store energy. They are used as well for small electronic devices as for electric cars or the storage of renewable energies. Due to the increasing demand of such batteries, it is important to develop

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and study mathematical models in order to understand the charging and discharging process. During the last years it was observed that the classical battery models (like e.g. a shrinking core model) do not predict the right behavior for lithium-ion batteries [1].

As an alternative to the classical models, Singh et al. [2] and Zeng et al. [3] proposed to use an extended phase-field model of Cahn-Hilliard or Cahn-Larché type. Their idea bases on the fact that LiFePO4 has the strong tendency to separate in a lithium rich and a lithium poor phase. The model takes inherently care of the intercalation reactions at the phase boundaries. Singh et al. and Zeng et al. introduced a non-linear Newton boundary condition for the chemical potential reflecting the chemical reactions on the surface using generalized Butler-Volmer kinetics. That model is sometimes called Cahn-Hilliard reaction (CHR) model. The fundamental difference to the classical Cahn-Larché model is the new chemically active boundary condition instead of the classical no-flux condition.

In recent years, the classical Cahn-Larché model describing phase-separation in elastic materials was studied intensively. In particular, the existence, the uniqueness, the regularity and the long-time behavior of solutions were investigated (see [4, 5] and the references therein). Often the main idea for the analysis was to write the equations as an H^{-1}-gradient flow. This bases essentially on the mass conservation of the solution which allows proving a priori estimates. However, in the CHR model the mass will not be conserved in general due to the chemical reactions at the boundary. For this reason, our approach to handle the CHR model analytically is to use a non-quadratic dissipation potential and to introduce a corresponding generalized gradient structure instead of the H^{-1}-gradient structure (see [6, 7] for details on generalized gradient structures). This ansatz naturally takes into account the non-linear Newton boundary condition and circumvents the analytical problem with the non-conserved mass. To the best of our knowledge, this additional structure of the CHR model was not known before.

In [8] and [9], the Cahn-Larché model was expanded to describe also damage of an alloy using a scalar damage variable z. The damage is driven by a rate-dependent dissipation potential. Assuming that the damage process is unidirectional and that the damage variable lies in a fixed interval, i.e. $[0,1]$, we are confronted with the mathematically challenging task to deal with inequality constraints guaranteeing $\partial_t z \leq 0$ and $z \in [0,1]$. In the context of lithium-ion batteries, the charging behavior is expected to depend strongly on the damage of the material. For this reason we include such a damage variable in the CHR model [2, 3]. The main objective of this work is to prove the existence of a weak solution of this coupled model. As in [9], we are also able to deal with the physically meaningful gradient term $|\nabla z|^2$ in the damage energy density (see [10]). Hence, we do not need to restrict to $|\nabla z|^p \, (p > \text{space dimension})$.

During the last years, many damage models based on the model of Frémond and Nedjar [11] describing damage in concrete (see also [10]) were investigated. The models divide basically in two types, the rate-independent [12–14] and the rate-dependent models [8, 9, 15, 16]. Both types can be coupled with different other equations to describe e.g. different phases [8, 9], inertia [17] or thermal effects [18–21].